MSTe NEWS

Fall 2020
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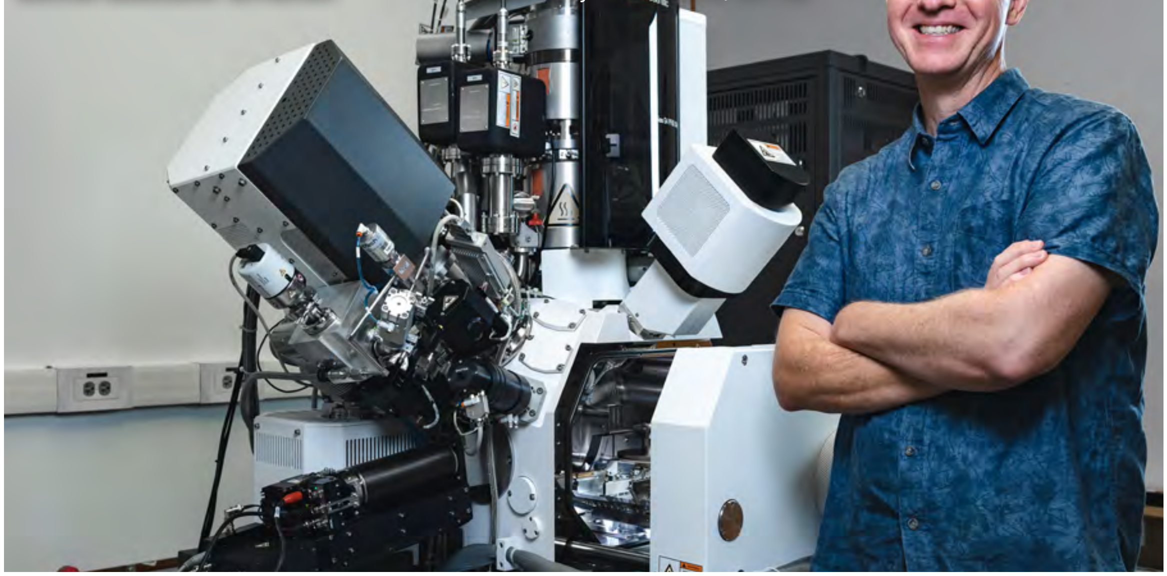
INSIDE



Rod McCabe with the newest addition to the Electron Microscopy Laboratory, the plasma focused ion beam (PFIB), which combines a xenon plasma FIB with scanning electron microscopy, energy dispersive x-ray spectroscopy, and electron backscatter diffraction. Photos by Kevin Sutton, XIT-TSS

Rod McCabe

"At Los Alamos, McCabe has characterized metals that span the periodic table from beryllium to uranium—one of his favorites due to its unique metallurgical properties."

Zooming in to get the big picture on materials performance

Honing in on the details is important in Rod McCabe's line of work. As a materials scientist he uses the tools and capabilities of the Los Alamos Electron Microscopy Laboratory (EML) to examine and distinguish the features of metal microstructures.

His results are used to further understanding and are aimed at connecting how a material's structure influences its properties and performance under specific conditions. The work is part of the Lab's goal to reliably predict a material's performance over its lifetime and design properties that were previously unattainable.

As part of a Basic Energy Sciences-funded project focusing on hexagonal-close-packed metals, McCabe contributes to an effort aimed at better understanding how materials deform and ultimately fail. The outcome of this project, which relies on a "close working relationship between modelers and experimentalists," McCabe said, "will be better-informed models for the strength and failure of materials." Such information "is essential for developing materials with improved properties," he said—such as materials that are stronger, lighter, or more ductile.

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Los Alamos National Laboratory NATIONAL LABORATORY EST.1943

From Ellen's desk . . .

Dear MST,

As we just closed the fiscal year, I have been reflecting on the state of the division, and in particular, the health of our budget, staffing plans, and infrastructure. As many of you know, the division has grown in both budget and workforce. Since 2018, the division has grown from 150 to 174 permanent staff (but note, with students, post docs, and contractors—we are a division of 218). As one might imagine, our budget has grown significantly too. In 2018, at year end, we had a budget of $85 million. While I am still collecting some final numbers, all projections indicate that we closed out FY20 at $115 million. This growth has occurred primarily in our applied energy programs as well as Pu Sustainment. However, it is important to note that there have been important contributions to this growth across much of the portfolio, including in our OES, BES, and LDRD programs.

With that said, to support this programmatic growth, as a division we have done a tremendous amount of hiring to grow while outpacing attrition. At the same time, we have been establishing numerous new capabilities at TAs -3, -35, and -55. While this is exciting, it means we have some things to carefully consider. We have had numerous capability investments (i.e., new microscopes at TAs -3 and -55, new mechanical testing capabilities at TAs -3 and -35, and new synthesis capabilities across the division). But we are starting to feel the real crunch of the limitations of our aging facilities. Still more, even with this substantial growth, we continue to hire. And I believe that we really need to spend time thinking about mentoring, career development, and retention of our most important investment—our staff.

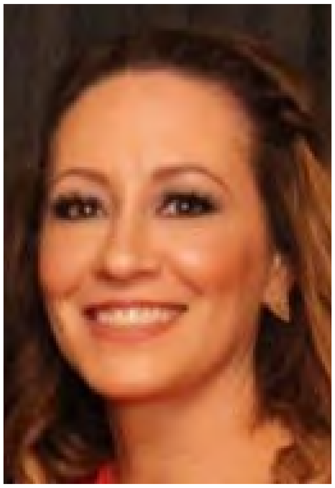
"... the division office has dedicated considerable time this year to making sure that staff are recognized for their achievements through nominations for promotions as well as NNSA/DOE and professional society recognitions."

To this end, MST-DO, your group offices, and ALDPS have been working to address some of these issues. With regard to infrastructure, we were pleased to be part of the PEI-1 completion at TA-55 and staff in MST-16 are working hard toward completion of REI-1. This fall we have started to examine the upgrades that are going to be needed if the TFF at TA-35 is going to be an enduring facility. While these projects—along with some changes to our work-from-home policy—may help with some of the congestion in our work spaces, I know more investment is going to be required. That is why I am looking forward to working with the ALDPS Deputies Council regarding planning for the Future Materials Campus at LANL.

As mentioned above, hiring, mentoring, career development, and retention are also going to be critically important for the division's success. To this end, MST-DO has been engaged in a few activities this past year. First, the division office has hired a staff operations manager, Rachel Morse. Rachel will have a leadership role in guiding staffing, workforce development, and university engagement in MST. Second, as a division, we have already started to examine career development offerings for our staff and first versions of these have been offered with a mentoring workshop in September and an opportunity for technicians working at TA-55 to participate in a pilot program to work toward an associate's degree through ALDWP's NEST program. Finally, the division office has dedicated considerable time this year to making sure that staff are recognized for their achievements through nominations for promotions as well as NNSA/DOE and professional society recognitions. But the work here is only beginning and more options for career development will have to be considered if we are going to provide growth opportunities for all of our staff. In FY21, I am looking forward to building on this track record and addressing an even broader swath of the needs within the division.

As MST-DO works through these important topics, I am thinking through how to best collect data to help focus our efforts and be most effective. One recent initiative of particular interest is reviewing and acting upon information gathered for the ALDPS culture survey. I will likely be using the Virtual Coffee framework as a platform for collecting input from all of you. As such, please look for and participate in these forums.

Happy New Fiscal Year!
Ellen



From Rachel's desk . . .

“While it is unfortunate that the opportunity for face-to-face meetings will be a little more difficult, I look forward to introductions and dialogue with you and encourage you to reach out.”

Dear MST,

It is with great enthusiasm that I joined MST-DO in late September and it is an honor and privilege to serve as staff operations manager, formerly known as chief of staff, for the division. I want to take this opportunity to introduce myself and provide you with background on my experience and my focus areas in this position. Like most of you have experienced recently, I too have faced the challenges of primary work from home status, schooling children at home, and adapting through all of the changes that have come with the pandemic. While it is unfortunate that the opportunity for face-to-face meetings will be a little more difficult, I look forward to introductions and dialogue with you and encourage you to reach out.

I joined LANL in July 2001 as an administrative assistant (AA) for ESA Division. Prior to that, I was a contractor working for what was then called Personnel Security, now known to most of you as Clearance Processing. My time spent in these positions gave me a broad perspective of not just the inner workings of a group office, but my time in clearance processing gave me an extensive overview of the Laboratory. In both positions, I established a network across LANL. Following my time as an AA in ESA, I gained valuable experience as a professional staff assistant (PSA) supporting the weapons mission in ALDW. Specifically, I spent nine years in the role supporting the detonator design mission in Q-6. This opportunity afforded me the experience and knowledge to provide effective assistance to the group in its operations. I subsequently transitioned to ISR-DO as chief of staff and then joined M Division as chief of staff, in its previous iteration of Explosive Science and Shock Physics. As noted above, I have gained valuable experience in the group office setting and recognize that it helped shape my career.

I welcome any and all opportunities to engage with you. In my new role in the division, I intend to focus on some of my many passions, including creating efficiencies in our work and communications approaches, clearing roadblocks for staff to help facilitate the critical technical work you were hired to do, developing our staff, and nurturing our student pipeline.

Thank you for the opportunity to serve you all and stay well.

MST Staff Operations Manager
Rachel Morse

McCabe cont.

Working at different length scales, the researchers are studying deformation twinning and an important deformation mechanism in these metals. The work, which leverages McCabe's expertise in electron microscopy, has resulted in several journal publications, including a 2020 *Science Advances* paper, and has implications for the transportation and nuclear industries.

At Los Alamos, McCabe (Materials Science in Radiation and Dynamics Extremes, MST-8) has characterized metals that span the periodic table from beryllium to uranium—one of his favorites due to its unique metallurgical properties. He is a member of MST-8's dynamic and quasi-static loading modeling team.

McCabe initially considered a career as a mechanical engineer and worked in the semiconductor industry before returning to school to earn his PhD in materials science and engineering. Materials was a minor aspect of his undergraduate degree, he said, but as a field on its own it "is the fascinating study of why materials have certain properties and how to affect those properties through changing the microstructure." In addition, "we get to use mind-blowing, world-class instruments to study these materials, such as electron microscopes, neutron diffraction, and x-ray synchrotrons."

The enthusiasm McCabe brings to linking diverse materials properties is also apparent in his role managing the EML, which connects him with researchers across the Laboratory. According to McCabe, the most exciting aspect of this "is interacting with the users, learning about all of the various types of research at LANL that take advantage of electron microscopy, and helping users obtain the best data possible from our tools."

The plasma focused ion beam is used for various characterization and testing applications including transmission electron microscopy specimen preparation, 3D serial sectioning, and micromechanical specimen cutting and testing with cutting rates around 20-50 times faster than a traditional focused ion beam.

McCabe joined Los Alamos in 2000, drawn by the opportunity to perform materials science research and development in the Mountain West region of the United States, an area that has "beautiful weather, a plethora of outdoor activities, a relative dearth of people, and family on my doorstep," he said. "At LANL, I have opportunities to collaborate with experimentalists and modelers of a large range of expertise to study basic materials problems and applied science and engineering issues fundamental to our national security."

By Renae Mitchell, CEA-CAS

Rod McCabe's favorite experiment

What: Automatic twin statistics from electron backscattered diffraction (EBSD) data

Why: Large-scale experimental statistics of the dependence of twinning on microstructure allow for improved physics in crystal plasticity models

When: 2009

Where: Los Alamos's Materials Science Laboratory

Who: Rodney McCabe, Peter Marshall, Gwenaelle Proust, James Rogers (all MST-8)

How: We developed code to take EBSD data as input and output statistical twinning dependencies.

The "a-ha" moment: There were no "a-ha" moments in the code development. Rather we tried different rules to see what worked. There have been several "a-ha" moments using the code to examine statistical twinning tendencies ever since.

Staff recognized for distinguished performance

For their essential contributions to the Lab's mission, several members of MST were recognized with 2019 Distinguished Performance Awards.

Every year, the awards recognize individuals and teams who have distinguished themselves in pursuit of this mission through outstanding scientific, technical, operational, community service, and/or administrative contributions. Awardees supported the Laboratory Agenda by improving operations, overcoming technical obstacles, and using innovative approaches to solve problems.

MST staff were members of the following large teams receiving awards this year.

SuperCam Mars-Rover instrument team:
Keith White (Nuclear Materials Science, MST-16)

Plutonium science team: Carlos Archuleta, Christopher Baxter, Matthew Curtis, Ryan Fulcher, Meghan Gibbs, Austin Goodbody, Benjamin Hollowell, Jay Jackson, Karl Krenek, Georgette Maestas, Todd Martinez, Tomas Martinez, Daniel Olive, Alison Pugmire, Michael Ramos, Silas Romero, Robert Sykes, Paul Tobash, Keith White, Clarissa Yablinsky (all MST-16); and Saryu Fensin (Materials Science in Radiation and Dynamics Extremes, MST-8).

Tri-lab tantalum strength team: Shuh-Rong Chen, Saryu Fensin, George Gray, and David Jones (all MST-8). ■

Blas Uberuaga named APS Fellow

Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MST-8) has been named a 2020 American Physical Society (APS) Fellow.

He was nominated in the APS Division of Computational Physics. His citation is for "the development of accelerated molecular dynamics methods and their application to the understanding of radiation effects in materials, including the amorphization resistance of complex oxides, and the discovery of a new mechanism for point defect recovery at interfaces."

Uberuaga is the radiation science modeling team leader in MST-8. He is also the director of FUTURE (Fundamental Understanding of Transport Under Reactor Extremes), an Energy Frontier Research Center funded by the Office of Basic Energy Sciences (BES). His primary expertise is the simulation of materials at the atomic scale, particularly the dynamics of defects. He has been involved in the development of advanced computational and simulation methods to characterize kinetics in materials (nudged elastic band and accelerated molecular dynamics). He has applied this expertise to understanding radiation damage in materials, with a particular focus on complex oxides and nanostructured materials.

As part of FUTURE, he is also considering the synergies between irradiation and corrosion in determining material evolution in reactor environments. He leads two other projects: an internal project on scintillator discovery and another BES project focused on the relationship between the chemical ordering within oxides and the kinetics of atoms.

Uberuaga, who has a PhD in physics from the University of Washington, has more than 250 peer reviewed technical publications (>18000 citations, h-index of 49) and nearly 100 invited presentations.

Technical contact: Blas Uberuaga ■

Integrated approach accelerates nuclear fuel development and qualification

A novel strategy exploiting advanced modeling and simulation techniques and leveraging existing capabilities promises to transform nuclear fuel development and qualification.

In research appearing in *Journal of Nuclear Materials*, Christopher Stanek (Materials Science in Radiation and Dynamics Extremes, MST-8) and external collaborators outline a process integrating advanced modeling and simulation tools with separate-effects testing. This "co-design" technique, which combines experiment with modeling, enables integral fuel performance analyses resulting in decreased time for developing and qualifying a new fuel system as well as associated costs.

"The enthusiasm associated with the concept of accelerated fuel qualification is exciting," Stanek said. "That there was such a good turnout at a recent (pre-COVID-19) event on Capitol Hill highlighting the idea, with participation from a Congressman and key Nuclear Regulatory Commission staff, industry, and DOE researchers is encouraging."

The approach is a departure from the experimental trial and error method intrinsic to the historic paradigm, which typically required more than 20 years to go from a new integral fuel concept to one qualified and approved by a regulator for deployment.

The coupling of experiment with advanced modeling and simulation, including sensitivity analyses and uncertainty quantification, can accelerate the development of new fuel concepts, expand their operational envelope, and reduce the dependence on exhaustive integral testing.

"The next steps converting the vision described in this paper to reality are critical," Stanek said. According to the researchers, this process, which enables innovation in the nuclear industry, is the best way to modernize and accelerate cost-effective research, development, and deployment of high-performance, safer nuclear fuel technologies. Increasing the urgency in adopting this method is the limited number of experimental nuclear facilities that allow for separate-effects or integral irradiation testing of nuclear fuels. This also highlights the need to recapitalize these facilities to support the high volume of small-scale tests necessary to inform integral fuel performance modeling.

The work leverages Los Alamos's decades of expertise in and capabilities for modeling, simulation, and post-irradiation examination materials studies.

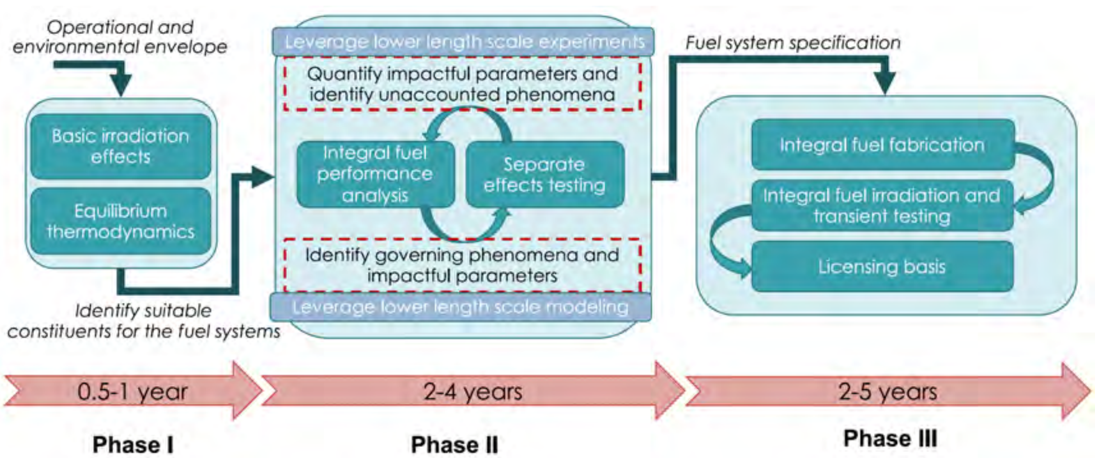
"LANL has a key role to play in both the computational and experimental elements of this important initiative," Stanek said.

The research was funded by the DOE Office of Nuclear Energy, jointly under the Advanced Fuels Campaign and Nuclear Energy Advanced Modeling and Simulation programs. The work supports the Laboratory's Energy Security mission area and the Materials for the Future science pillar.

Reference: "Accelerating nuclear fuel development and qualification: Modeling and simulation integrated with separate-effects testing," *Journal of Nuclear Materials* 539, 152267 (2020).

Researchers: Christopher Stanek (MST-8); Kurt A. Terrani, Nathan A. Capps, Andrew T. Nelson (Oak Ridge National Laboratory); Matthew J. Kerr, Steven L. Hayes (Idaho National Laboratory); Christina A. Back (General Atomics); Brian D. Wirth (University of Tennessee).

Technical contact: Christopher Stanek



The process workflow for accelerated fuel qualification consists of three distinct phases, as illustrated above. The information generated and the decisions made at the end of each phase guide and orient the subsequent work to efficiently reach a successful outcome. Advanced modeling and simulation methods made available only within the past decade are at the core of this approach to facilitate constituent and system selection in Phase I, produce functional integral fuel performance designs in Phase II, and provide the licensing basis in Phase III.

Ion sputtering's role examined in quest to develop atomic resolution images of plutonium

Actinide scientists broadly regard plutonium (Pu) as the most complex element in the periodic table. Its reactivity, radioactivity, and toxicity make plutonium intriguing—yet challenging—to analyze.

With the aim of characterizing Pu surfaces with high spatial resolution, Los Alamos developed a first-of-its-kind scanning tunneling microscopy (STM) capability for plutonium housed in an ultra-high vacuum (UHV) system. Despite the tool's ability to produce atomic resolution images of well-known standards, achieving such resolution for Pu sample surfaces has been prevented by the difficult challenge of producing a suitable Pu surface.

Sputtering is a well-established method of preparing Pu surfaces under UHV conditions for analysis. However, no studies have addressed the effects of this method on the surface roughness of Pu. Although it is well known that sputtering of a sample surface can result in damage and roughening, when combined with annealing in certain materials under the right conditions, sputtering can result in atomically clean, smooth, and defect-free surfaces.

As part of an effort to produce Pu surfaces of the quality needed for atomic resolution STM imaging, Los Alamos researchers investigated the effects of argon-ion sputtering and subsequent annealing on the surface roughness of Pu samples. According to Miles Beaux, who led the effort to establish the capability, "Direct observation of the radioactive decay of a single atom using STM was proposed in 2003 by Alexander V. Balatsky and Jian Xin Zhu [LA-UR-03-4350]. The establishment of a plutonium capable STM is an opportunity to reach this objective."

Their research revealed that such sputtering/annealing cycles progressively increased the surface roughness of the Pu. Additionally, Auger and STM measurements revealed an initially unstable and dynamically changing surface that became increasingly stable as sputter/anneal cycles were applied. The stabilized surface region contained within the sputter crater was observed to be unchanged for up to 17 months after the final sputter anneal cycle. This was surprising since it was assumed that under UHV conditions, the material would revert back to its pretreated state.

The *Journal of Nuclear Materials* published the work.

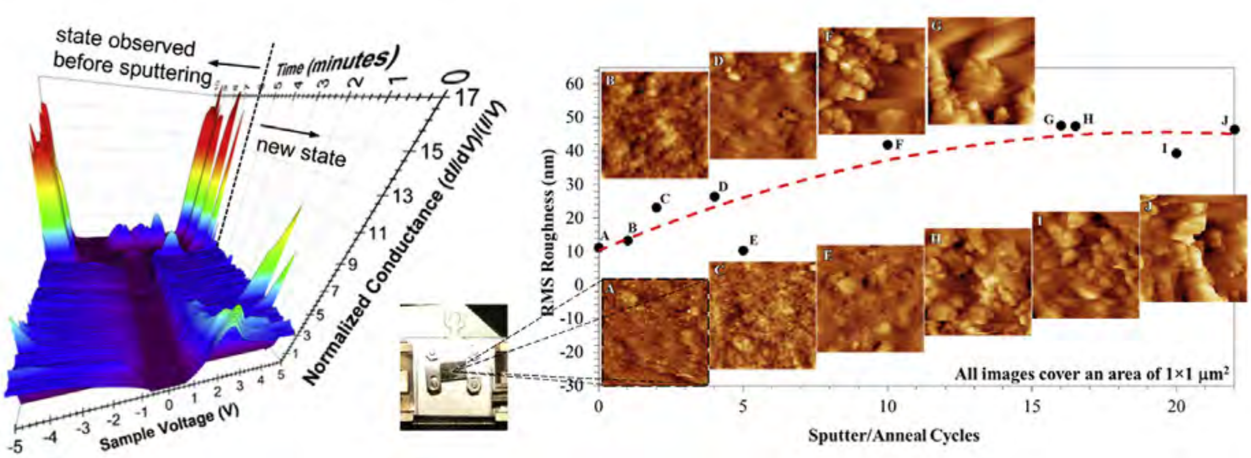
The work was performed in the Plutonium Surface Science Laboratory, which is operated as a collaboration between Engineered Materials (MST-7) and Nuclear Materials Science (MST-16).

The work, which supports the Laboratory's Stockpile Stewardship mission area and the Materials for the Future science pillar, was funded by the Lab's Science Campaign 1.

Reference: "Effects of ion sputtering on plutonium surfaces," *Journal of Nuclear Materials* 540, 152378 (2020).

Researchers: Miles Beaux, Igor Usov (MST-7); and Stephen Joyce (Physical Chemistry and Applied Spectroscopy, C-PCS). Samples used in this work were provided by MST-16.

Technical contact: Miles Beaux ■



A picture of the plutonium sample is shown (center) with microscope images (right) of the sample surface. The spectral graph (left) demonstrates the dynamically changing electronic structure of the plutonium surface over 10 minutes after the first sputter treatment.

Left: Scanning tunneling spectra collected over a 10-minute duration from a location within a 0.5 x 0.5 nm² area on the same electropolished Pu sample after the first sputter/anneal treatment. Right: STM images of the electropolished Pu sample with the root mean square roughness values for each image plotted as a function of sputter/anneal cycles.

Heads UP!

Target Fab marks 5S + Safety success

Residents of the Target Fabrication Facility (TFF) have embraced the 5S + Safety process, treating an entire lab space to the housekeeping process—and elsewhere collaborating with subject matter experts in an ongoing effort. The results are organized work areas, efficient work processes, and increased safety.

Leading the way were members of Engineered Materials' (MST-7) thin films and coatings team. Igor Usov, Miles Beaux, Bryan Bennett, Alexander Edgar, Victor Siller, Douglas Vodnik, Camille Wong, and Dali Yang have organized their experimental labs, which are used to fabricate and characterize thin films and coatings in support of multiple LANL programs.

The team identified, separated, and sorted their tools. They set in order items by frequency of use. To help standardize the space, they created tags so all team members can easily identify items stored in cabinets and workbenches and on countertops. This encouraged the team to also inspect their tools for safety and integrity. They are now able to quickly locate and retrieve the necessary tools for each process outlined in their integrated work documents. The team also created a clearly defined Life Safety Protection Zone. This emergency/safety area within the laboratory includes a shower, fire extinguisher, waste-spill kits, eye-wash station, personal protection equipment, and signage at entry and exit ways.

In sustaining their success, team members weekly apply quality assurance, 5S, and human performance improvement practices to their work, laboratory, and office cleanups. The team's newly hired postdoctoral researchers and research technicians have also incorporated these habits into their routines. The team has even on occasion bolstered 5S efforts elsewhere in TFF, giving a shine to areas such as the dock, transportainers, and shared common spaces.

Miquela Sanchez (MST-7), Edward Freer (Science and Technology Operations, MSS-STO), and members of Fire Protection (ES-FP) are collaborating on two 5S + Safety projects underway in the TFF's penthouse. In tackling the engineer's mechanical desk, they have sorted mechanical, electrical, and plumbing blueprints and in the process determined if they need to be scanned for retention. They have also collaborated with craft workers to sort and unpack—and ensure protocol is followed in removing and recycling—heavy piping, equipment, insulation, and other infrastructure and packing materials. These efforts have helped keep the penthouse free of debris, flammables, and chemicals—which is critical as the TFF's building automation system undergoes a $3 million, multi-year upgrade.

To learn how to apply the 5S + Safety method in your area, contact ALDPS 5S + Safety Champions Christie Davis (Sigma Division) and Jacki Mang (LANSCE Facility Operations).

For more information see int.lanl.gov/org/ddste/aldps/5s-safety/index.shtml. ■

Steps to 5S + Safety

Sort: Decide what is needed and eliminate the unneeded items.

Set in order: Arrange and identify necessary items for ease of use.

Shine: Clean the workplace and keep it clean.

Standardize: Create consistency by identifying and applying standards.

Sustain: Maintain 5S + Safety and establish ways to preserve the work area.

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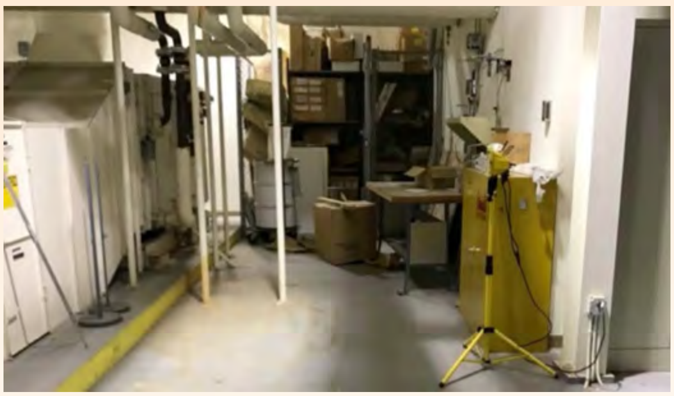
HeadsUP cont.

Toolboxes are labeled, enabling staff to easily locate needed items.



The Target Fabrication Facility penthouse is now free of debris, flammables, and chemicals—which is essential as the building's HVAC system is being upgraded

The engineer's desk in the Target Fab penthouse was stacked with blueprints to be sorted through and scanned if being retained.

Celebrating service

Congratulations to the following MST Division employees who recently celebrated a service anniversary:

John Joyce, MST-16 .... 30 years
James Valdez, MST-8 .... 25 years
Franklin Fierro, MST-7 .... 20 years
Sven Vogel, MST-8 .... 20 years
Alice Smith, MST-16 .... 15 years
David Jones, MST-8 .... 5 years
Christopher Matthews, MST-8 .... 5 years

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To submit news items or for more information, contact Karen Kippen, ALDPS Communications, at 505-606-1822 or aldps-comm@lanl.gov.

For past issues, see www.lanl.gov/org/ddste/aldps/mst-e-news.php.

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NNSA National Nuclear Security Administration